Session #16: Homework Solutions

Problem #1

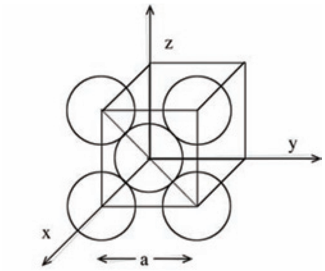
For the element copper (Cu) determine:

(a) the distance of second nearest neighbors.

(b) the interplanar spacing of {110} planes.

Solution

(a) The answer can be found by looking at a unit cell of Cu (FCC).



Nearest neighbor distance is observed along <110>; second-nearest along <100>. The second-nearest neighbor distance is found to be “a” (Another way of finding it is looking at LN4, page 12).

Cu: atomic volume $= 7.1 \times 10^{-6}\ m^3$ / mole $= \frac{N_A}{4} a^3$ (Cu: FCC; 4 atoms/unit cell)

$$a = \sqrt[3]{\frac{7.1 \times 10^{-6} \times 4}{6.02 \times 10^{23}}} = 3.61 \times 10^{-10}\ m$$

(b) $d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + 1^2}}$

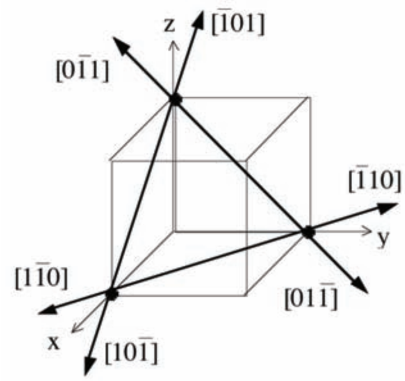
$$d_{110} = \frac{3.61 \times 10^{-10}}{\sqrt{2}} = 2.55 \times 10^{-10}\ m$$

Problem #2

Consider a (111) plane in an FCC structure. How many different [110]-type directions lie in this (111) plane? Write out the indices for each such direction.

Solution

Let's look at the unit cell.



There are six [110]-type directions in the (111) plane. Their indices are:

$$\left(10\bar{1}\right),\ \left(\bar{1}01\right),\ \left(\bar{1}10\right),\ \left(1\bar{1}0\right),\ \left(0\bar{1}1\right),\ \left(01\bar{1}\right)$$

Problem #3

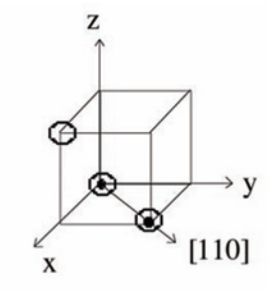
Determine for barium (Ba) the linear density of atoms along the <110> directions.

Solution

Determine the lattice parameter and look at the unit cell occupation.

Ba: BCC; atomic volume = 39.24 cm^3/mole; n = 2 atoms/unit cell

$$3.924 \times 10^{-5} \left(m^3\ /\ mole\right) = \frac{N_A}{2} a^3$$



$$a = \sqrt[3]{\frac{2 \times 3.924 \times 10^{-5}}{6.02 \times 10^{23}}} = 5.08 \times 10^{-10}\ \text{m}$$

$$\text{linear density} = \frac{1\ \text{atom}}{a\sqrt{2}} = \frac{1}{5.08 \times 10^{-10} \times \sqrt{2}}$$

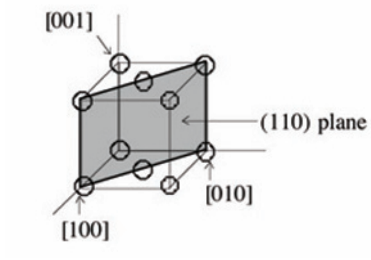
$$= 1.39 \times 10^{9}\ \text{atoms/m}$$

Problem #4

For aluminum at 300K, calculate the planar packing fraction (fractional area occupied by atoms) of the (110) plane and the linear packing density (atoms/cm) of the [100] direction.

Solution

Aluminum at 300K has FCC structure:



Volume unit of a cell:

$$V = \frac{10\ cm^3}{mole} \times \frac{1\ mole}{6.02 \times 10^{23}\ atoms} \times \frac{4\ atoms}{1\ unit\ cell}$$

$$= 6.64 \times 10^{-23}\ cm^3\ /\ unit\ cell$$

$$V = a^3 \rightarrow a = \left(6.64 \times 10^{-23}\ cm^3\right)^{1/3} = 4.05 \times 10^{-8}\ cm$$

For FCC: $\sqrt{2}a = 4r \rightarrow$ atomic radius $r = \frac{\sqrt{2}}{4}a = \frac{\sqrt{2}}{4}\left(4.05 \times 10^{-8}\ cm\right)$

$$= 1.43 \times 10^{-8}\ cm$$

Planar packing fraction of the (110) plane:

area of shaded plane in above unit cell = $\sqrt{2}a^2$

number of lattice points in the shaded area = $2\left(\frac{1}{2}\right) + 4\left(\frac{1}{4}\right) = 2$

area occupied by 1 atom = πr^2

$$\text{packing fraction} = \frac{\text{area occupied by atoms}}{\text{total area}} = \frac{2\pi r^2}{\sqrt{2}a^2}$$

$$= \frac{2\pi\left(1.43 \times 10^{-8}\ cm\right)^2}{\sqrt{2}\left(4.05 \times 10^{-8}\ cm\right)^2} = 0.554$$

Linear packing density of the [100] direction:

$$\text{density} = \frac{1\ \text{atom}}{a} = \frac{1\ \text{atom}}{4.05 \times 10^{-8}\ cm} = 2.47 \times 10^7\ \text{atoms/cm}$$

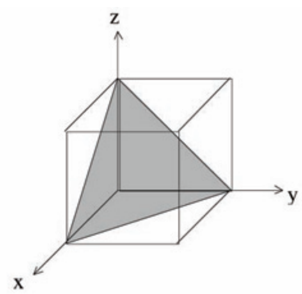
Problem #5

Sketch a cubic unit cell and in it show the following planes: (111), (210), and (003).

Solution

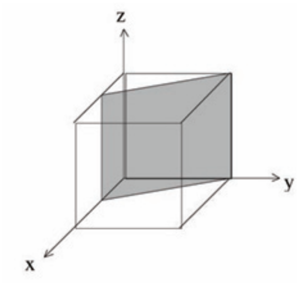
(111) inverse = $\frac{1}{1}\ \frac{1}{1}\ \frac{1}{1} \rightarrow x = 1, y = 1, z = 1$

This plane intersects x-axis at x = 1, y-axis at y = 1, z-axis at z = 1



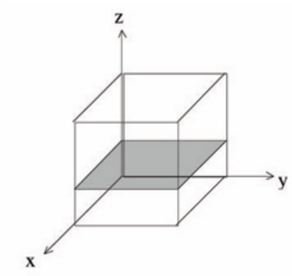
(210) inverse = $\frac{1}{2}\ \frac{1}{1}\ \frac{1}{0} \rightarrow x = 1/2, y = 1, z = \text{infinity}$

This plane intersects x-axis at x = 1/2, y-axis at y = 1, and does not intersect the z-axis.



(003) inverse = $\frac{1}{0}\ \frac{1}{0}\ \frac{1}{3} \rightarrow$ x = infinity, y = infinity, z = 1/3

This plane does not intersect either the x-axis or y-axis, and intersects the z-axis at z = 1/3.

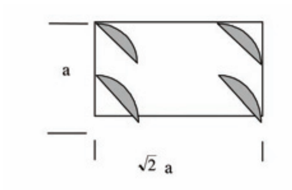


Problem #6

Braquium (Bq) is simple cubic. Calculate the atomic density (atoms/cm^2) in the (011) plane of Bq. The molar volume of Bq is 22.22 cm^3.

Solution

(011) looks like this:



4 x $\frac{1}{4}$ atoms = 1 atom

area = $\sqrt{2}a^2$

$$\frac{1}{a^3} = \frac{N_A}{V_{molar}} \rightarrow a = \left(\frac{22.23}{6.02 \times 10^{23}}\right)^{1/3} = 3.33 \times 10^{-8} \text{ cm}$$

$$\therefore \text{ atomic density} = \frac{1}{\sqrt{2}a^2} = 6.376 \times 10^{14} \text{ atoms/cm}^2$$

Problem #7

(a) What are the coordinates of the largest interstitial hole in the FCC structure? (Hint: where should we put an extra atom if we were looking for the most room?)

(b) How many of these sites are there per unit cell?

Solution

(a) The largest "holes" are the octahedral voids formed by eight (8) contiguous atoms, for example, around the center of an FCC unit cell. The location of the center is therefore: 1/2, 1/2, 1/2.

(b) Where are the octahedral voids in the unit cell? One in the center, and ¼ void centered on each edge. Since there are 12 edges, we have a total of (1 + 12/4) = 4 octahedral voids in an FCC cell.

Problem #8

What is the family of planes {hkl} with an interplanar spacing of d = 1.246 Å in nickel (Ni) with a = 3.524 Å?

Solution

We know: $d_{(hkl)} = \dfrac{a}{\sqrt{h^2 + k^2 + l^2}}$

$$\sqrt{h^2 + k^2 + l^2} = \frac{a}{d_{(hkl)}} = \frac{3.524}{1.246} = 2.828$$

$$h^2 + k^2 + l^2 = 8 = (2^2 + 2^2 + 0)$$

The family of planes is {220}